

Phase diagram of the one-dimensional, two-channel Kondo lattice model

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(Dated: February 2, 2008)

Employing the density matrix renormalization group method and strong-coupling perturbation theory, we study the phase diagram of the $SU(2) \times SU(2)$ Kondo lattice model in one dimension. We show that, at quarter filling, the system can exist in two phases depending on the coupling strength. The weak-coupling phase is dominated by RKKY exchange correlations while the strong-coupling phase is characterized by strong antiferromagnetic correlations of the channel degree of freedom. These two phases are separated by a quantum critical point. For conduction-band fillings of less than one quarter, we find a paramagnetic metallic phase at weak coupling and a ferromagnetic phase at moderate to strong coupling.

PACS numbers: 71.27.+a, 75.20.Hr, 75.30.Mb, 75.40.Mg

Although Landau's theory of Fermi liquids is one of the cornerstones of modern condensed matter physics,¹ many materials show metallic properties that do not fit into this framework. For instance, it is well known that one-dimensional systems usually behave as Luttinger liquids rather than Fermi liquids.² In higher dimensions, the proximity of a quantum critical point (QCP) is considered to be responsible for the non-Fermi liquid properties of systems like $CeCu_{6-x}Au_x$.³ The quadrupolar Kondo effect has been proposed as an alternative source of non-Fermi liquid behavior. This effect is described by the two-channel Kondo model^{4,5}. This model has a non-Fermi liquid ground-state because of frustration in the screening of a localized impurity by two degenerate conduction electron channels if the degeneracy of the channels M is greater than twice the impurity spin S .⁶ The single-impurity two-channel Kondo model can provide an adequate description of dilute systems like $Th_{1-x}U_xRu_2Si_2$ ⁷ or $Y_{1-x}U_xPd_3$,⁸ but it does not incorporate the lattice effects that become relevant in fully concentrated compounds like UBe_{13} .⁵ These materials are described by the two-channel Kondo lattice model (KLM).

In this paper, we address the question of what happens when two of these fundamental sources of non-Fermi liquid behavior coincide. For this purpose we study the $SU(2) \times SU(2)$ Kondo lattice model in one spatial dimension. The Hamiltonian reads

$$H = -t \sum_{i m \sigma} \left(c_{i m \sigma}^\dagger c_{i+1, m \sigma} + \text{H.c.} \right) + \frac{1}{2} J \sum_{i m \alpha \beta} \mathbf{S}_i \cdot \left(c_{i m \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} c_{i m \beta} \right),$$

where $t > 0$ is the conduction electron hopping amplitude, taken to be the same in both bands, and $c_{i m \sigma}^\dagger$ ($c_{i m \sigma}$) creates (annihilates) an electron on lattice site i , $1 \leq i \leq L$ (L being the number of lattice sites), with channel flavor $m = +$ or $-$ and spin projection $\sigma = \uparrow$ or \downarrow . The Heisenberg spin operator for the localized f -electrons

($S_i = \frac{1}{2}$) is defined by $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha \beta} f_{i \alpha}^\dagger \boldsymbol{\sigma}_{\alpha \beta} f_{i \beta}$, where the f -operators satisfy the constraint $f_{i \uparrow}^\dagger f_{i \uparrow} + f_{i \downarrow}^\dagger f_{i \downarrow} = 1$ and $\boldsymbol{\sigma}$ is a vector of Pauli spin matrices. The conduction band filling is defined as $n_c = n_{c+} + n_{c-} = (N_{c+} + N_{c-})/L$ with $N_{c\pm}$ the number of conduction electrons in channel $m = \pm$, respectively; $n_c = 1$ corresponds to the quarter filled system. The KLM may be derived from the more fundamental periodic Anderson model in the limit of strong Coulomb repulsion where the Kondo coupling is usually antiferromagnetic (AF), $J > 0$,⁹ or alternatively in the "extended Kondo limit".¹⁰ In the following, we measure all energies in units of t .

Not much is known about the ground-state phase diagram of the two-channel KLM. Tsvelik and Ventura¹¹ investigated this model using a mean-field analysis and found that at half filling the system exists in two phases. One is dominated by RKKY exchange interaction effects, and the other by Kondo screening. A QCP separates these two regimes. A generalized one-dimensional two-channel KLM with an additional Heisenberg interaction, J_H , between the f -spins was studied by Andrei and Orignac.¹² In the limit of strong J_H , they find that the system is in a superconducting phase with odd-frequency singlet pairing of the electrons. In infinite spatial dimensions, the ground state is characterized by superconducting or magnetic phases, which may coexist or compete.¹³

The focus on the *two*-channel system below or at quarter filling is also motivated by the relation to the *single*-channel system at half filling or less. In particular, the quarter-filled case for the two-channel model is analogous to the half-filled case for the single-channel model in that there is one conduction electron per impurity spin, which leads to complete screening at strong coupling. In the following, we will show that the situation in the two-channel model *below* quarter filling is qualitatively similar to the single-channel case below half filling, while exactly at quarter filling it is quite different. The phase diagram of the single-channel model is well understood, at least qualitatively.^{14,15} In the low carrier limit, this system

displays ferromagnetic order with *complete* polarization, $S_{\text{tot}} = (L - N_c)/2$, where $n_c \ll 1$.^{16,17} In the strong-coupling limit, the ground state is ferromagnetic for all n_c .¹⁸ Exactly at half filling, the single-channel model is known to be a Kondo insulator.^{15,19} This is a quantum disordered phase in which the conduction electrons are bound into local singlet states with the impurity spins, and both the spin and charge correlation functions decay exponentially in space and time.

In order to calculate the ground-state properties of the one-dimensional two-channel KLM, we use the finite-system algorithm²⁰ of the DMRG to calculate gaps, equal-time correlation functions, and the total spin of the ground state. We keep up to 1000 states per block on lattices of up to $L = 50$ sites and obtain a maximum discarded weight of 10^{-5} . Fig. 1 shows the total spin S_{tot} per site extrapolated to the thermodynamic limit for various couplings and conduction electron densities. Here S_{tot} is calculated directly by taking the expectation value of $\mathbf{S}_{\text{tot}}^2$ in the ground state and also by examining the degeneracy of excited states in various S_z sectors. A finite-size extrapolation is then used to determine whether $S_{\text{tot}} = (L - N_c)/2$ (complete ferromagnetism), $S_{\text{tot}} < (L - N_c)/2$ but finite (incomplete ferromagnetism), or $S_{\text{tot}} = 0$ (paramagnetism) in the thermodynamic limit. At quarter filling ($n_c = 1$), the nature of the ordering is also indicated for $S_{\text{tot}} = 0$ phases.

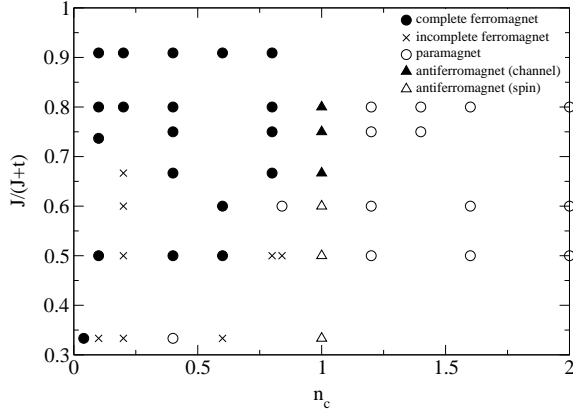


FIG. 1: Ground-state phase diagram of the two-channel KLM as a function of conduction band filling n_c . The AF channel- and spin-ordered phases at quarter filling are associated with a singlet ground state. The crosses indicate polarizations that extrapolate in the thermodynamic limit to values between 25% and 90% of complete polarization.

Fig. 1 shows a large region of complete ferromagnetism for $n_c < 1$ above a certain critical value J_c which decreases with decreasing n_c and tends to zero as $n_c \rightarrow 0$. In the completely polarized phase, each conduction electron forms an itinerant singlet with the f -spins. Delocalization of these singlets leads to ferromagnetic ordering of the remaining unscreened f -spins. The complete polarization for all J at low conduction electron density is in agreement with an exact argument¹⁶ for a single con-

duction electron. For $J < J_c$, there is a region of incomplete ferromagnetism, similar to one that has been found in the periodic Anderson model.²¹ While we cannot rule out that this region is due to a continuous transition to the complete ferromagnetic phase, the local spin profiles in the incomplete ferromagnetic regime show small ferromagnetic domains (corresponding to polarizations between 25% and 90% of the complete value), suggesting that phase separation may occur here. For $n_c \geq 1$, we find a singlet ground state for all couplings J .

Exactly at quarter filling, we find two phases as a function of J . At weak coupling ($J \lesssim 2.0$), the electrons of different flavors generate independent RKKY interactions between the localized moments. We observe strong correlations of the f -spins at a wave vector $q = \pi/2$, as in the single-channel model at *quarter* filling.²² At stronger coupling ($J \gtrsim 2.0$), the system is in a channel AF phase, where the correlations of the channel degree of freedom decay as $1/r$. The two phases are separated by a QCP.

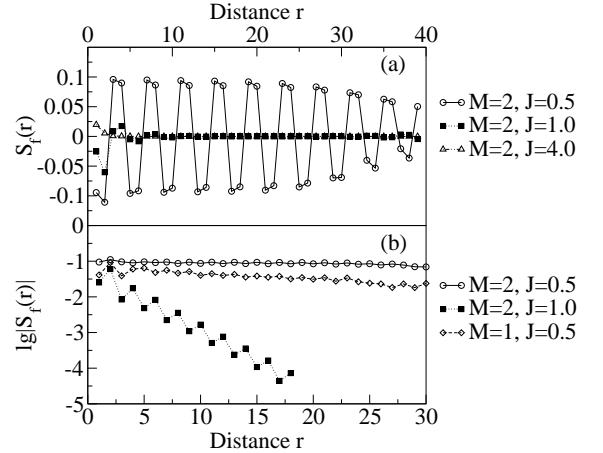


FIG. 2: Magnetic correlation function $S_f(r) = \langle S_z(0)S_z(r) \rangle$ of the f -spins for the two-channel KLM at $n_c = 1$ in (a) and for the single- and two-channel models, both at quarter-filling, in (b).

Fig. 2(a) shows that in the two-channel model the spin-spin correlation function decays slowly for weak coupling ($J = 0.5$ or 1.0) and is short-ranged for strong coupling ($J = 4.0$), i.e., numerically zero for more than two lattice spacings. The transition between the two behaviors occurs at $J \approx 2.0$ (not shown in Fig. 2), where the correlations extend over roughly two lattice sites. Fig. 2(b) shows a comparison between the spin-spin correlations functions $S_f(r)$ of the single-channel and two-channel KLM on a logarithmic plot. The ground state for $M = 1$ in the weak-coupling limit shows RKKY liquid behavior with spatial oscillation characterized by a wave vector $q = \pi/2$. In the $M = 2$ case the correlations at $J = 0.5$ decay so slowly that the asymptotic behavior cannot be determined for the system sizes considered, as can be seen in Fig. 2(b). At larger J -values [e.g., $J = 1.0$ in Fig. 2(b)], the correlation functions appear to decay exponentially, consistent with the opening of a gap in the

spin excitation spectrum due to the transition into the channel-ordered phase. Fig. 3 shows the magnetic structure factor $S_f(q)$ for the two-channel system. The amplitude of the peak at $q = \pi/2$ (the wavevector expected for a RKKY liquid) becomes smaller with increasing J , indicating that the magnetic correlations between the f -spins become weaker and finally vanish at $J \approx 2.0$.²³

It is known that the RKKY correlations of the single-channel KLM at *quarter* filling become unstable with increasing coupling toward a ferromagnetic ground state.^{15,24} However, the two-channel model cannot be ferromagnetic at quarter filling because each f -spin is screened by an electron, so that some other kind of symmetry breaking must lift the degeneracy of the ground state. Fig. 4 shows the staggered magnetization $D(r)$ of the channel degree of freedom, with

$$D(i-j) = \sum_{\sigma\sigma'mm'} m m' \langle n_{im\sigma} n_{jm'\sigma'} \rangle.$$

where $n_{im\sigma} = c_{im\sigma}^\dagger c_{im\sigma}$. In Fig. 4(a) one sees that $D(r)$ decays with $1/r$ as function of the distance $r = i-j$ for $J = 4.0$. Fig. 4(b) shows that the AF channel correlations become stronger with increasing coupling and the quasi-long-range behavior develops for $J \gtrsim 2.0$.

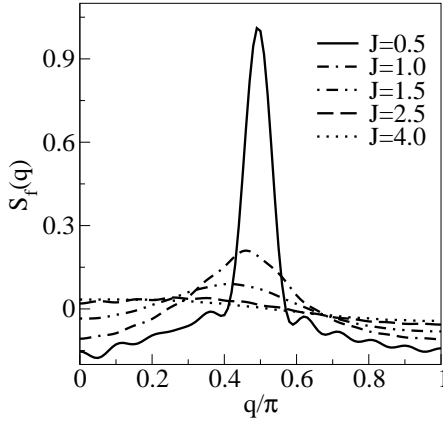


FIG. 3: Magnetic structure factor of the two-channel KLM model as a function of wavevector q for various J at $n_c = 1.0$.

In order to understand our numerical results for strong coupling, we use the methods of Ref. 18 to derive an effective Hamiltonian valid for $t/J \ll 1$. At $n_c = 1$, the channel flavor is the only degree of freedom and the low-energy spectrum can be described by a pseudospin-1/2 model. Accordingly, the effective Hamiltonian is a Heisenberg model for the channel spin,

$$H = \frac{16t^2}{3J} \sum_i \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_{i+1}, \quad (1)$$

where $\boldsymbol{\tau} = \frac{1}{2} \sum_{mm'} b_{im}^\dagger \boldsymbol{\sigma}_{mm'} b_{im'}$ is defined in terms of hard-core bosons

$$b_{im}^\dagger = \frac{1}{\sqrt{2}} (c_{im\uparrow}^\dagger f_{i\downarrow}^\dagger - c_{im\downarrow}^\dagger f_{i\uparrow}^\dagger), \quad (2)$$

which represent local Kondo singlets. In one spatial dimension, model (1) has been solved exactly using the Bethe ansatz.²⁵ The ground state is characterized by critical AF correlations that decay as $1/r$, in agreement with our numerical findings at quarter filling [see Fig. 4(a)]. This critical behavior is replaced by long-range AF ordering for $D > 1$. Due to the SU(2) pseudo-spin invariance of H , the AF ordering is present for all three $\boldsymbol{\tau}$ -components. In particular, the order along the z axis corresponds to staggered orbital ordering while the x, y -ordering gives rise to a Bose-Einstein condensation of excitons (particle-hole singlet bound states between the two channels).

For $n_c < 1$, the low-energy subspace in the strong-coupling limit contains states with zero and one conduction electron per site. While the local state with one conduction electron can be described by the hard-core bosons of Eq. (2), the empty state acquires spin-1/2 character from the f spins. It can therefore be represented as a constrained fermion $\varphi_{i\sigma}^\dagger = (1 - n_i^b) f_{i\sigma}^\dagger$, with $n_i^b = \sum_m b_{im}^\dagger b_{im}$. At strong coupling, the effective Hamiltonian has the form

$$H_0 = -\frac{t}{2} \sum_{i\sigma,m} \left(b_{im}^\dagger \varphi_{i\sigma}^\dagger \varphi_{i+1,\sigma}^\dagger b_{i+1,m} + \text{H.c.} \right).$$

In analogy to the infinite- U Hubbard model, the ground-state wavefunction can be written as a direct product of a charge, spin, and orbital component

$$\begin{aligned} |\psi_n\{\tau; \sigma\}\rangle &= |n_c\rangle \otimes |\tau_1 \cdots \tau_{L-N}\rangle \otimes |\sigma_1 \cdots \sigma_N\rangle \\ &= \sum_{i_1 < i_2 < \cdots < i_N} \Gamma_{i_1 i_2 \cdots i_N}^{(n)} \varphi_{i_1 \sigma_1}^\dagger \cdots \varphi_{i_N \sigma_N}^\dagger b_{j_1 \tau_1}^\dagger \cdots b_{i_{L-N} \tau_{L-N}}^\dagger |0\rangle \end{aligned}$$

where $\{\tau; \sigma\} = (\tau_1, \dots, \tau_{L-N}; \sigma_1, \dots, \sigma_N)$ and $|0\rangle$ denotes the vacuum of φ and b particles. The complete spin degeneracy of H_0 in the strong coupling limit is lifted in $\mathcal{O}(t^2/J)$. The effective Hamiltonian in this order contains only one term that lifts this degeneracy:

$$H_1 = \frac{t^2}{2J} \sum_{i\sigma,m} \left(\varphi_{i+1,\sigma}^\dagger b_{i+1,m} n_i^\varphi b_{i-1,m}^\dagger \varphi_{i-1,\sigma} + \text{H.c.} \right),$$

where $n_i^\varphi = \sum_\sigma \varphi_{i\sigma}^\dagger \varphi_{i\sigma}$. Here H_1 exchanges two spins by hopping of a fermion over another to an empty next-nearest-neighbor site. In the same way as for the single-channel KLM, it can be shown that the off-diagonal elements of H_1 are all non-positive and the Hamiltonian matrix in real-space is completely connected. The Perron-Frobenius theorem (see, for instance, Ref. 26) then states that the ground state is unique and that the coefficients of the wave-function can be chosen to be strictly positive. The only spin state that has strictly positive coefficients in each of the subspaces of H_1 is the one with maximum total spin. Therefore, the ground state of the two-channel KLM below quarter-filling is ferromagnetic in the strong-coupling limit, in accordance with our numerical findings.

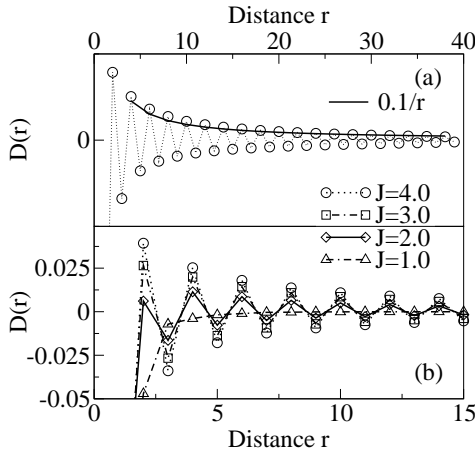


FIG. 4: Staggered magnetization $D(r)$ for the channel degree of freedom for various J at quarter filling ($n_c = 1.0$). The longer distance behavior for $J = 4.0$ (where there is a slower falloff, approximately $\propto 1/r$) is shown in (a) and a shorter range in r is shown for all four J -values in (b).

In this paper, we have mapped out the zero-temperature phase diagram of the two-channel KLM as a function of conduction band filling n_c and Kondo coupling strength J . Our main results are that the phase diagrams of the two-channel and single-channel KLMs are

qualitatively similar for low band fillings ($n_c < 1$ in both models) but quite different at $n_c = 1$. For $n_c < 1$, the addition of a second degenerate band of conduction electrons does not alter the physical picture of the single-channel model if n_c is low or J is large. The similarity between the two phase diagrams for $n_c < 1$ further suggests that the metallic ground state of the two-channel KLM at weak coupling is determined by two *independent* Kondo effects in both channels. In contrast, at quarter-filling ($n_c = 1$) the two-channel KLM exhibits a quantum phase transition between this metallic phase and an insulator characterized by strong AF correlations of the channel degrees of freedom. Our perturbative analysis shows that this insulating phase is present for any spatial dimension D and has long-range ordering for $D > 1$. Therefore, we also expect a QCP separating the metallic and the insulating phase for $D > 1$. The AF channel (or excitonic) fluctuations diverge at the QCP and can produce a deviation from the normal Fermi-liquid behavior of the metallic state. In this way we see that the deviations from the Fermi-liquid behavior which are obtained in the dilute (impurity model) and the concentrated (lattice model) limits have a common origin in the fluctuations of the channel degree of freedom.

T.S., D.L.C., and C.D.B. acknowledge support from U.S. Department of Energy.

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